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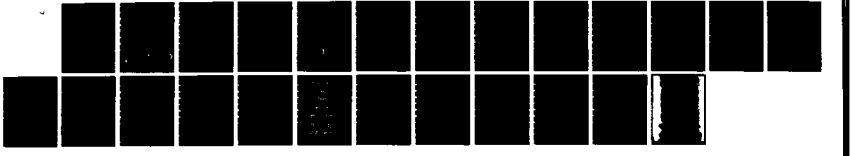

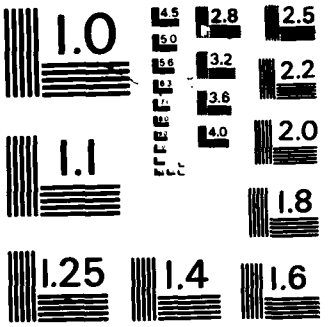

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Numerical Simulations of the Structure and Propagation of Self-Sustained Detonations

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Two-dimensional time-dependent numerical simulations have been performed to determine a computational method of determining the natural cell size of a self-sustained detonation. The systematic approach developed involves simulating systems with tube heights both larger and smaller than the transverse cell spacing. This approach, tested on a mixture of hydrogen, oxygen and argon, provided us with an estimate of the cell size which is in excellent agreement with experimental observations. The simulations also provided insight into some aspects of the mechanism by which a self-sustained detonation propagates. The evolution of the curvature of the transverse wave appears to be the crucial feature. Depending on the curvature of the transverse wave at the time of its reflection from either a neighboring transverse wave or a wall, the cell is either flattened or pockets of unreacted gas can be formed.

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Numerical Simulations of the Structure and Propagation of Self-Sustained Detonations

CONTENTS

NUMERICAL SIMULATIONS OF THE STRUCTURE AND PROPAGATION OF SELF-SUSTAINED DETONATIONS

I. INTRODUCTION

The propagation of self-sustained gaseous detonations is a complex, multi-dimensional process involving interactions between incident shocks, Mach stems, transverse waves and boundaries of the regions through which the detonation is moving[1,2,3]. The triple points formed at the intersection of the transverse wave with the Mach stem and the incident shock trace out the patterns we call detonation cells[1,4,5]. Extensive experimental data[6,7,8] has shown that the size and regularity of this cell structure is characteristic of the particular combination of initial material conditions, such as composition, density and pressure[1,9,10]. Theoretical efforts[6,11,12,16] to explain the cell size vary in accuracy and in some cases predict sizes within a factor of two[2]. Numerical simulations have shown that these cells can be formed by perturbing a planar one-dimensional detonation, but they also show some dependence on initial conditions[13]. Here we present a computational study of self-sustained detonations with emphasis on finding a systematic computational method to estimate the natural cell size for a particular material. In addition, by examining the behavior of the transverse wave structure, we have been able to develop insight into the mechanism of propagation of self-sustained detonations.

We have concentrated on planar mode detonations, which are two-dimensional and unsteady in the neighborhood of their detonation fronts. They are obtained experimentally in tubes of narrow, rectangular cross section when the preferred transverse wave spacing of the detonation is at least five times the width of the tube[1,6]. This study extends the ideas and methods described at the 19th Combustion Symposium[14] in which a time-dependent two-dimensional numerical model[15] was used to study the formation of unreacted gas pockets within the detonation

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cell of a marginal detonation. In the simulations discussed in this paper, we perturb a planar propagating detonation, i.e., one without any initial transverse structure, with a large pocket of unburned material behind the detonation front. First we show that the burning of a large enough pocket provides a sufficient perturbation to the planar detonation to cause it to form a multi-dimensional structure. This is an equilibrium configuration[16] since it repeats exactly at equally spaced intervals as the detonation propagates down the channel. It is also an unique structure since changing the size and orientation of the initial perturbation does not affect the final state. We then describe a procedure for determining the detonation cell size from such numerical simulations based on systematically increasing the tube height in the computation. In this way a relatively limited set of calculations can give an estimate of the cell size from a first principles calculation. This approach has provided us not only with an estimate of the detonation cell size, but also with a picture of the role played by the transverse wave in a self-sustained detonation. Finally, the set of calculations described below has allowed us to put into perspective the previous calculations of the formation of unburned gas pockets behind detonation fronts.

II. THE NUMERICAL MODEL

The numerical model used to perform the simulations described in this paper solves the time-dependent conservation equations for mass, momentum and energy[17] in two dimensions using one variant of the Flux-Corrected Transport (FCT) algorithm[18]. This model with various initial and boundary conditions has been used to study single and double Mach reflections[19], mixing and vortex formation at material interfaces[20] and the formation of unreacted gas pockets behind propagating detonations[14,19]. Thus its ability to calculate complicated shock structures has been tested extensively against theory, experiment and independent computations.

In addition to the solution of the convection terms by FCT, we have included an induction parameter model which is a phenomenology develcped to reproduce the correct ignition delays and subsequent energy release due to chemical reactions[15]. In this model three quantities must be specified: the time before any energy is released (the chemical induction time), the time it takes to release the energy, and the total amount of energy released. An induction parameter[15,21] is then defined which is a measure of how long the material has remained at a given temperature and pressure. In the calculations this quantity is convected with the fluid and is used to indicate when the available chemical energy should be released. For the supersonic reacting flows we are studying here, diffusive effects such as thermal conduction, viscosity and molecular diffusion are small. Thus we need to consider only the strong interaction between gas dynamics and chemistry. The convection and energy release algorithms are coupled by previously described methods[17].

In order to economically resolve the details of the flowfield behind the moving reactive shock front, an adaptive gridding method is used. A region of fine zones in the x-direction surrounds and moves with the shock front[15,17]. The remaining cells in the x-direction are evenly spaced, except that a smooth transition from fine to coarse zones is enforced. The cells in the y-direction are evenly spaced and have the same size as the fine zones in the x-direction. In the calculations described below, a 150 x 50 mesh was used which meant fine zones in the range 0.1 - 0.18 cm and coarse zones in the range 1.0 - 1.8 cm for the different systems simulated. Computational timesteps were in the range 0.1 - 0.18 microseconds. The calculations generally required 2000-3000 timesteps to reach an equilibrium detonation configuration. One calculation typically requires 90 minutes of CPU time on the Texas Instruments ASC computer.

III. RESULTS AND DISCUSSION

All the simulations described below were initialized by placing an elliptical pocket of unburnt gas behind a planar detonation propagating into a 65 torr (8.66 kPa), 298 K stoichiometric hydrogen-oxygen mixture diluted with 60% argon. Thus in these simulations the pockets are used as a device for initiating the perturbation. Tubes of 5, 7, 9 and 10 cm height were simulated.

Determination of Detonation Cell Size

The first calculation simulated a tube 5 cm high, which we estimated from the experimental data to be smaller than the natural detonation cell size of the mixture[1,7]. An unburnt gas pocket, placed symmetrically behind the planar detonation, generates pressure waves as it burns. These waves interact with the incident shock front causing the front to curve outwards and after a short time a portion of the incident shock reflects from the side walls of the tube. The transverse waves formed are strengthed due to collisions with each other and the walls, eventually forming the pair of well defined triple points seen in Fig. 1. This figure is a composite of seven "snapshots" of the density contours at intervals of 10 microseconds. In the first frame the transverse waves are moving away from each other and towards the wall, by the fourth frame they have reflected from the walls and are moving towards the center of the tube, and by frame 7 they are again moving towards the wall after colliding with each other. Small deviations in the contours in Fig. 1 at the symmetrical locations above and below the centerline are a result of small asymmetries in the calculation.

Figure 1 shows that the triple point structure does not immediately bounce off when it hits the wall, indicating that a complete detonation cell has not been formed. The pattern of the triple points for this calculation is clearer in Fig. 2A, which shows a time and space gap at the walls as the structure reforms.

Increasing the height of the tube to 7 cm, as shown in Fig. 2B, results in a considerably reduced gap in the path of the triple points propagating from the walls. Finally, the locus of the triple points for a 9 cm tube, shown in Fig. 2C, forms a complete detonation cell and what appears to be partial structures above and below it. From the figure we estimate the cell height and length to be about 8.5 cm and 19.6 cm, respectively.

Comparisons with Experimental Data on Detonation Cell Size

The predicted cell height or transverse wave spacing is in excellent agreement with estimates from experimental data as shown in Table I. Most of the experimental data available in the literature are for the rectangular mode of detonation propagation, that is, they were obtained in tubes in which the effect of the third dimension is significant. However, the work of Strehlow and co-workers[1,9] on the effect of tube geometry on preferred transverse wave spacing in a dilute stoichiometric hydrogen-oxygen-argon mixture provides an easy way of estimating the cell size for the mixture studied in the numerical simulations. Their study showed that for low pressures, the detonation cell size in the planar mode is larger than that in the rectangular mode by a factor of 2.0 to 2.5. Since the cell size for the rectangular mode of propagation in a 60% argon diluted stoichiometric hydrogen-oxygen mixture at 65 Torr is about 4 cm, we estimate the cell size for the planar mode to be about 9 cm. In addition to the published literature we have also compared the results to the experimental measurements of Edwards[27]. For a 60% dilute mixture, he obtained a cell size of 5.7 cm at 80 Torr and 10 cm at 60 Torr. This provides us with an estimate of 9 cm at 65 Torr, which is in quantitative agreement with the estimate from Strehlow et.al. These results have been summarized in Table I.

Table I

Detonation Cell Size for Stoichiometric Hydrogen-Oxygen Mixtures

Diluted with Argon

Dilution (%)	Mode of Propagation	Cell Size (cm)	Comments
0	Rectangular mode (3D)	2.0	Ref.(7)
50	Rectangular mode (3D)	3.0	Ref.(7)
70	Rectangular mode (3D)	5.0	Ref.(7)
70	Planar mode (2D)	11.5	Ref.(9,1)
60	Rectangular mode (3D)	4.0	Interpolated from Ref.(7)
60	Planar mode (2D)	9.0	Estimated from Ref.(7,9)
60	Planar mode (2D)	9.0	Interpolated from Ref.(27)
60	Planar mode (2D)	8.5	Calculated in this paper

Note: All the mixtures considered above are at an initial temperature and pressure of 298 K and 65 Torr.

Propagation of Self-Sustained Detonations

The surprising feature of the calculations shown in Figs. 2 is the flattened shape of the cell when the tube height is less than the cell height (e.g., Fig. 2A). Below we provide an explanation of this behavior based on observations of the temperature, pressure and density contours around the transverse wave structure. We also provide evidence that the varying cell shapes shown in Figs. 2A are a result of the shape and curvaturve of the transverse wave as it collides with the wall.

Figure 3 shows temperature contours from the 5 cm tube simulation at six different times at intervals of 10 microseconds. At cycle 2400 the transverse waves have already collided with each other and are moving towards the wall at an angle indicated by the arrows. It is useful to focus on the shaded region between the 1300 K and 2100 K contours since as it evolves it reflects the changing size of the induction zone. First we note the well-known fact that behind the transverse wave this region is very narrow and the 2100 K contour is close to the Mach stem. This is because the higher temperatures and pressures caused by the passage of the transverse wave decrease the size of the induction zone. Ahead of the transverse wave the region is much more extended behind the incident shock. Energy release behind a transverse wave generates pressure waves which drive it towards the wall. Thus the transverse waves are driven into the shocked but as yet unburned gas mixture ahead of it. This energy release also drives the Mach stem outward causing the characteristic bulge seen in the figures. This expansion causes a decrease in the velocity of the Mach stem and by cycle 2500 the reaction zone has begun to decouple from the Mach stem behind the transverse wave. By cycle 2600, the reaction zone is even more separated from the shock front. In the absence of walls, this separation would continue to grow until either the reaction zone and shock front became so decoupled that the detonation dies, or until ignition occurrs spontaneously due to heating for a long enough time in the induction region. This latter effect appears to occur in the 9 cm simulation described above in which triple points appear spontaneously in the induction zones just before reflection of the transverse waves from the walls. However, the detonation cell in this 5 cm case is re-initiated by the collision between the transverse waves and the walls. The collision reverses the direction of motion of the transverse waves and so the transverse waves again encounter shocked but unburned mixtures ahead of them. The transverse waves move towards each other and by cycle 2900 they have collided in the center of the tube. Again we observe a large induction zone beginning to form before the collision so that

when the transverse waves reverse direction they again encounter unburned material to propagate into.

This picture corroborates the rough criterion given by Fickett and Davis[2], who maintained that in a detonation cell, a large enough induction zone must form between two transverse waves receeding from each other. Then when the waves collide and their directions are reversed, they encounter enough unreacted material to sustain their propagation through to the next collision. Although this concept is supported by the calculations shown above, it does not give us a criterion for determining a cell size: we saw above that the 5 cm case is smaller than a detonation cell size, and yet we obtain a self-propagating repeatable structure.

To better understand the factors that determine the size of a cell, we must examine the curvature of the transverse wave as it reflects from the wall or another transverse wave. Consider the pressure contours for the 5 cm case shown in Fig. 4., in which the location of the transverse wave, incident shock and Mach stems are marked. For purposes of this explanation we call the 'head' of the transverse wave that portion at and close to the triple point, and we call the 'tail' that region of the transverse wave extending back towards the burned material. At cycle 3200 the transverse waves are moving towards each other, and we observe that the distance between the two heads is larger than the distance between the two tails. The pressure contours around the transverse wave outline its curvature. The same curvature is evident at cycle 3300, from which we conclude that the tails of the transverse waves are going to collide with each other earlier than the heads. Cycle 3600 is a time after the collision of the transverse waves at the center of the tube and the cell has been reinitiated. Comparing the figures here, we conclude that the curvature of the transverse wave is reversed at or around the time of collision. Also at cycle 3600, the heads of the transverse wave are closer to each other than the tails. Therefore the tails of the transverse wave collide with and reflect from the walls earlier than the heads. From

this we see that such reflection causes a higher pressure difference across the tail segment of the transverse wave as compared to that across the unreflected front segment. This high pressure region pushes the incident shock front forward and results in the flattened detonation cell we saw in Figs. 1 and 2A.

The above observations are for the 5 cm tube for which the natural detonation cell height is larger than 5 cm. Now consider the 7 cm case. Here the transverse wave can travel further, become weaker before collisions, and the inclination of the transverse waves to the tube walls is less. This is evident upon inspection of figures similar to Fig. 4 for the 7 cm case. If the height of the tube is exactly equal to the cell height, we expect the transverse wave to be parallel to the wall at the time of reflection and then every segment of it reflects from the wall at about the same time. The locus of the triple points in the 7 cm tube shown in Fig. 2B corroborates this argument since the gap in the path of the triple points almost disappears with the increase in the tube height. Furthermore, from the discussion above of the mechanism sustaining detonation propagation, we see that if the tube height is significantly larger than the detonation cell height, we expect generation of new triple points due to local instabilities occurring in the shocked material ahead of the transverse waves. This produces a new pair of transverse waves propagating towards the two transverse waves already present in the system. The new and old waves then collide with each other when the transverse wave spacing equals the detonation cell height. Therefore in a tube slightly larger than the detonation cell height we would observe four transverse waves at certain periods in the detonation cell cycle as well as a complete detonation cell within the tube. This is what is seen in Fig. 2C for the 9 cm simulation.

Formation of Unburned Gas Pockets

In the 9 cm tube case shown in Fig. 2C we also observed the presence of unburned gas pockets near the walls behind the detonation front[14,19]. The origin of these pockets in the calculation can be explained by extending the argument put forth above on the inclination of the transverse wave. Consider a case for which the tube height is slightly larger than the detonation cell height. In this case, a transverse wave moving towards the walls, which does not encounter another transverse wave moving in the opposite direction, continues to propagate though considerably weakened. However, here the head of the transverse wave reflects earlier than the rear segment. As previously discussed[14], this results in a portion of the gas near the head of the transverse wave burning first and effectively cutting off a gas pocket. For an unburned gas pocket to form in this way, ignition near the walls must be delayed by some effect. Thus an unburned pocket is more likely to occur in marginally detonable mixtures such as the one considered here or at the walls in real systems where there are heat losses.

Simulations with Asymmetric Initiation

A number of simulations were performed in which the initiating perturbing pocket was placed asymmetrically so that its axis was at an angle to the planar detonation front. In these cases unsymmetrical triple points evolved and disappeared quickly creating a very irregular cell structures. However, the system eventually evolved into the symmetrical cases and produced the cell structure shown in Figs. 2.

In another case we tried to take advantage of the symmetry about the centerline apparent in Figs. 2. In an earlier paper[14] we speculated that simulating a detonation in a tube which is half the cell height would force a half cell structure and be equivalent to half of a simulation of a full cell. To test this, we compared two calculations: a 10 cm tube in which a symmetrical pocket was used (similar to those in Fig. 2), and a 5 cm tube in which the upper half of a symmetrical

pocket was placed on the lower wall. The 10 cm calculation indeed verified the observations in the 9 cm case: a cell of about 8.5 cm was formed in the center of the system and there was not room enough for another full cell to appear in the calculation. The 5 cm case initially looked like the upper half of the 10 cm case, but as time went on it became irregular and eventually evolved into the regular structure shown in the 5 cm calculation in Fig. 2A. These results confirm that the equilibrium structures obtained in the numerical simulations are independent of the initial pertubations. From this we conclude that simulating half-cells can be misleading. Here we found in the 5 cm asymmetric simulation (which was the upper half of the 10 cm case) that two structures are vying with each other for dominance: one such as in Fig. 2A and another which is half of the 10 cm calculation. The dominant mode of propagation eventually wipes out the subdominant mode. These results are consistent with the ideas described above concerning the structure of the transverse wave at the time of reflection.

IV. SUMMARY AND CONCLUSIONS

The excellent agreement obtained between the numerical predictions and the experimental data on the detonation cell size show that the simulations described above present a systematic approach for numerically determining detonation cell sizes. The basic ingredients in such simulations are a model for the chemical kinetics and a convective transport algorithm that is accurate enough to resolve shocks, Mach structures, and reaction zones. The convective transport algorithm used here has been tested extensively and we understand its capabilities and limitations. The induction parameter model used for the chemical kinetics is a phenomenological model derived from a detailed chemical reaction rate mechanism. Such a parametric model has the potential of being useful in calculations such as these when either we cannot afford to use the full chemical reaction scheme or when such a scheme is not available but we have experimental data on ignition and

energy release times. However, the only way to benchmark the coupled models is by comparing to experiments and to calculations containing the detailed chemical rate scheme. With increased computational speed and memory available, we are close to being able to include a detailed chemical reaction model at least for hydrogen-oxygen combustion.

We also have found that the simulations are useful for graphically displaying the detailed, evolving structure of the detonation front. The results shown above have provided insight into some aspects of the mechanism by which a self-sustaining detonation propagates. They have indicated that the curvature of the transverse wave at the time of its reflection is extremely important to the resulting cell structure. First we observe in the simulations that the final result of a transverse wave collision is a reversal of the curvature of the transverse wave. This implies that the natural cell size might be defined as that distance between two triple points which occurs when the curvature of two oppositely moving transverse waves goes nearly to zero. This is substantiated by the evidence given above that if the tails of a transverse wave collide first, flattening of the cell occurs. Further, if the heads of the transverse waves collide first, an unburned pocket can form.

Future calculations will test several aspects of the results presented above. First, the approach for predicting cell sizes must now be tested for a wide range of hydrogen-oxygen mixtures, especially those whose detonation cell sizes are well-known from experiments. This should provide a better test of the validity of the induction parameter model for the chemistry, and tell us when and if we need more complete chemical models. Then calculations such as these with an induction parameter model can be applied to methane and other materials for which good chemical kinetic data exists. Finally, more resolved calculations must be done and the details of the structure and evolution of the transverse wave must be compared to previous observations[9, 22-26].

The observations presented of the structure are very convincing, but much more intermediate data is required for clarity and verification.

ACKNOWLEDGMENTS

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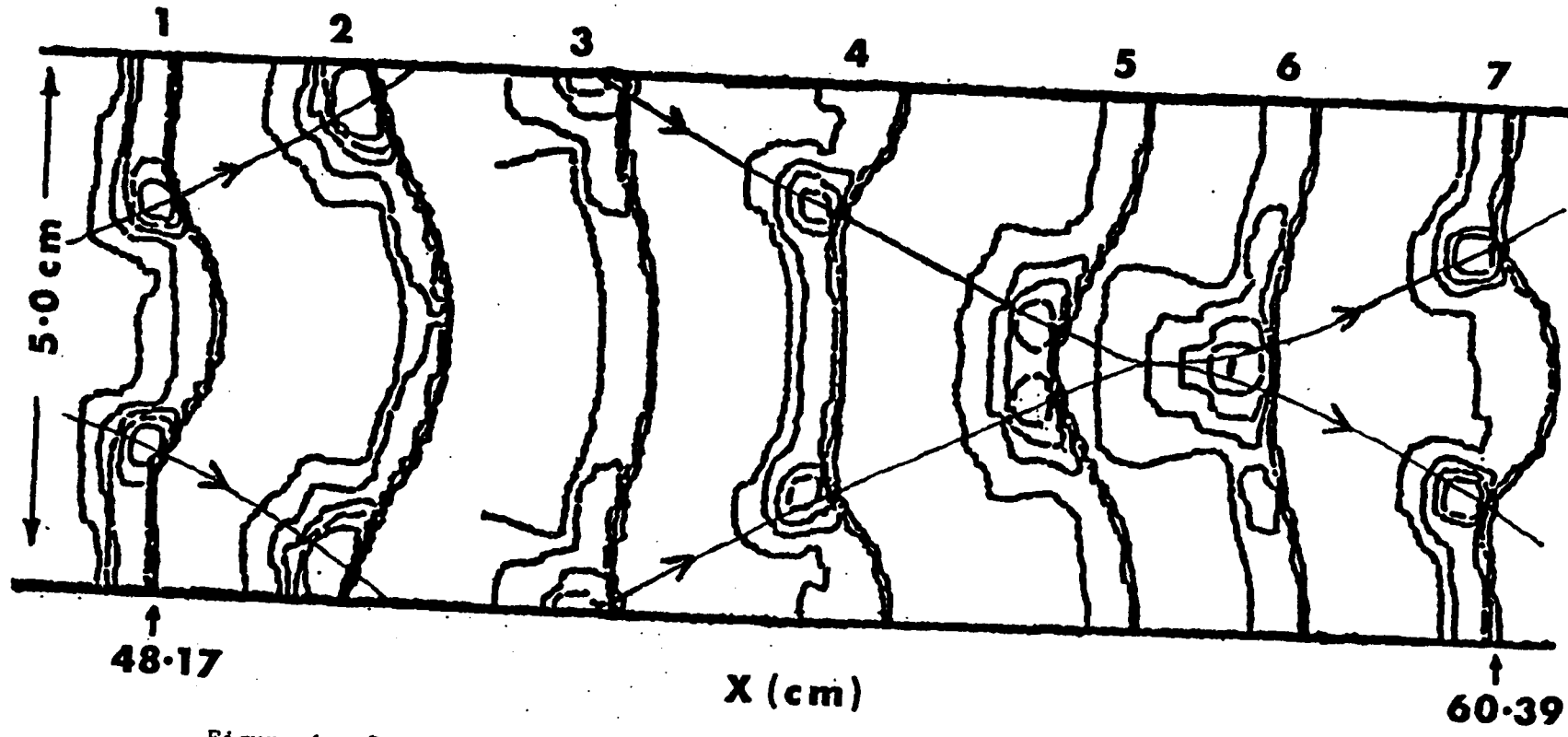

Figure 1. Composite of density contours from seven timesteps in the calculation of a propagating detonation in a hydrogen-oxygen-argon mixture in a 5 cm high tube. The direction of movement of the triple point is indicated by the lines with arrows.

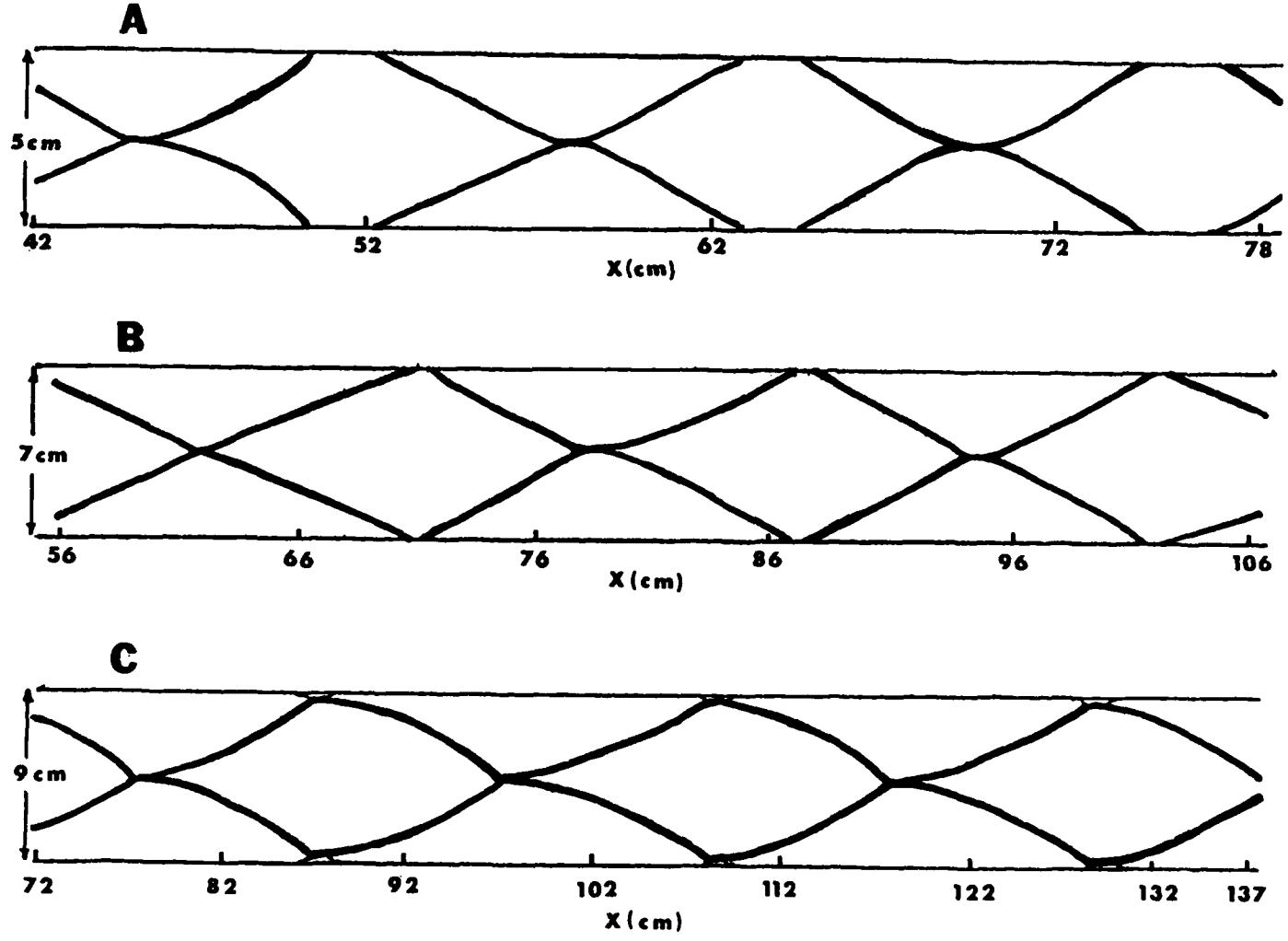

Figure 2. Calculated paths of triple points for the same mixture as in Figure 1. (A) 5 cm high tube. (B) 7 cm high tube. (C) 9 cm high tube.

TEMPERATURE CONTOURS

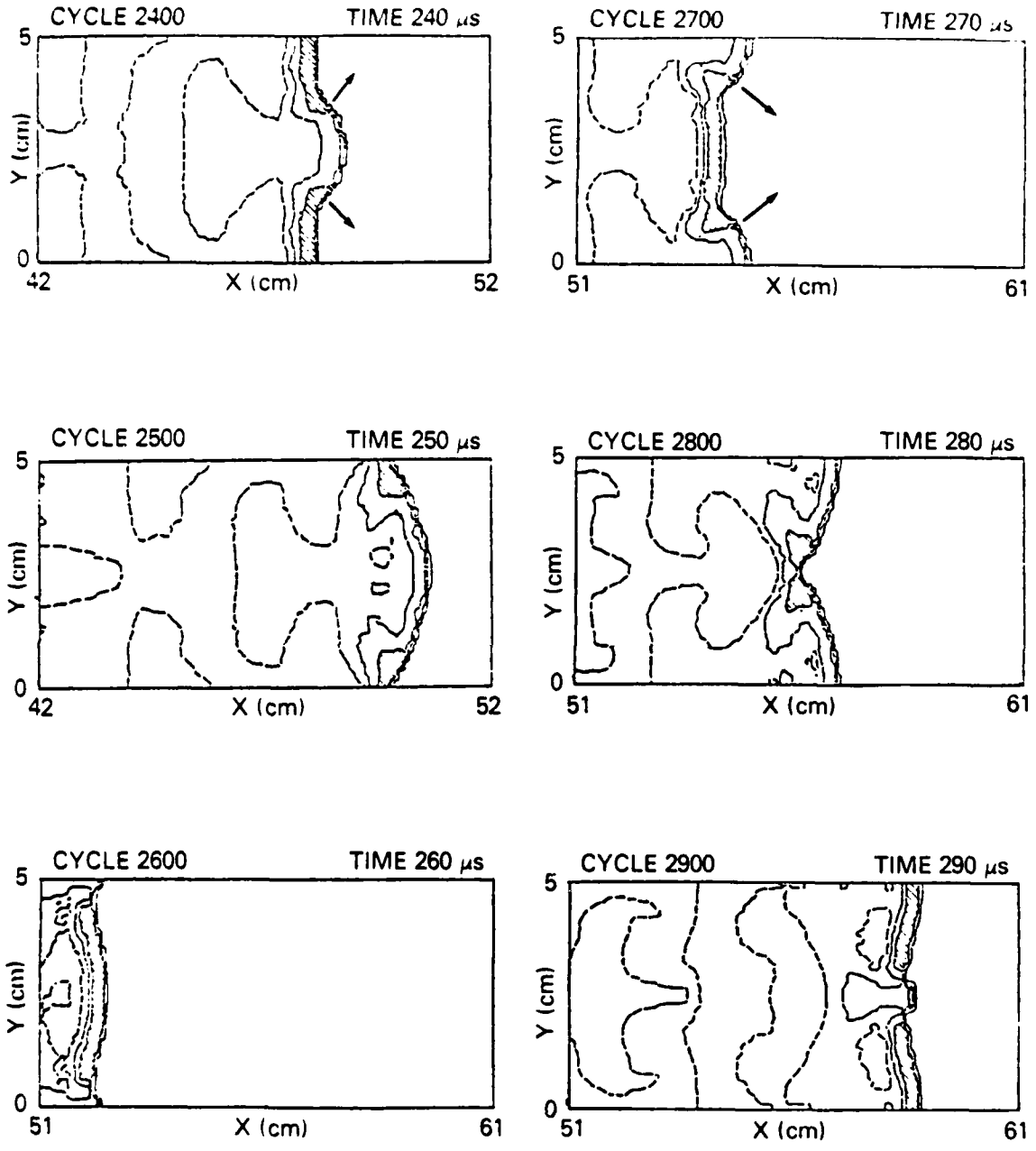

Figure 3. Temperature contours at six different times for the 5 cm tube calculation. The arrows indicate the direction of propagation of the triple points. The region between 1300 and 2100 K is shaded.

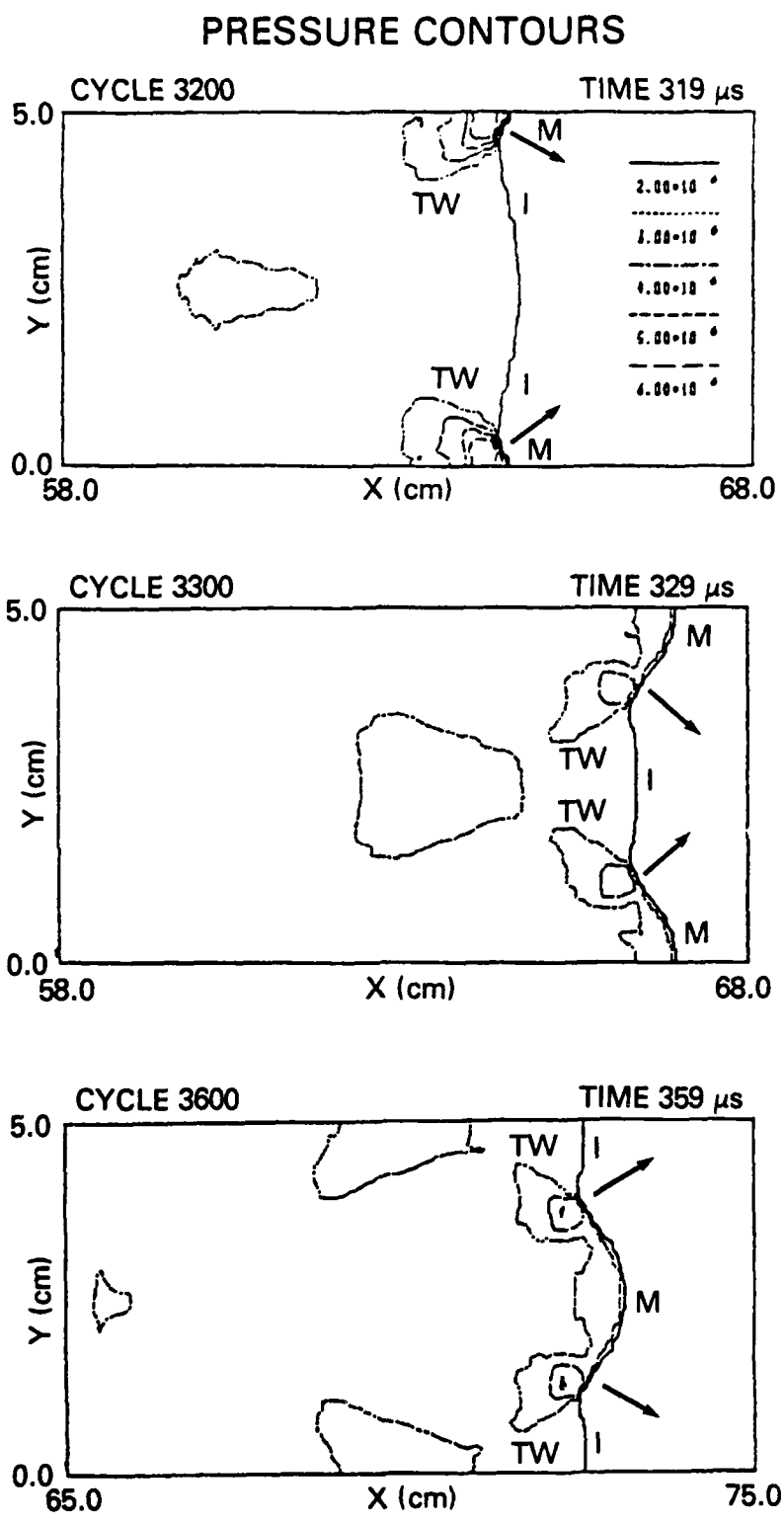

Figure 4. Pressure contours for the 5 cm tube calculation. The Mach stem, incident shock, and transverse waves are marked by M, I and TW, respectively.

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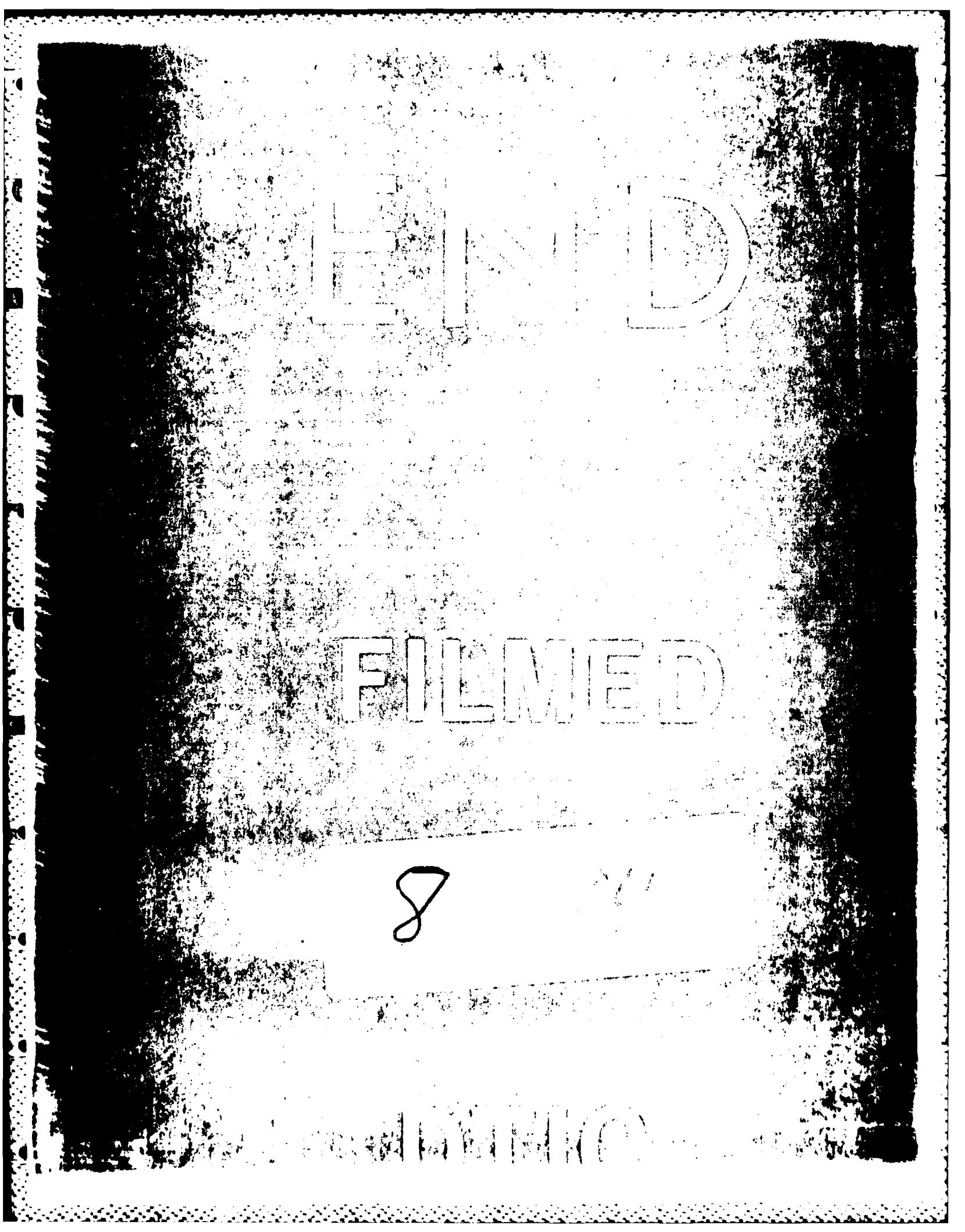
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